

Acetone

67-64-1 | DTXSID8021482

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 2.42

Global applicability domain: Inside

Local applicability domain index: 9.93e-01

Confidence level: 7.37e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Acetone</div> <div>Measured: 2.31</div> <div>Predicted: 2.42</div>	<div>Image not found</div> <div>Ethyl formate</div> <div>Measured: 2.19</div> <div>Predicted: 2.41</div>	<div>Image not found</div> <div>Propanal</div> <div>Measured: 3.02</div> <div>Predicted: 2.43</div>
<div>Image not found</div> <div>Methyl acetate</div> <div>Measured: 2.31</div> <div>Predicted: 2.41</div>	<div>Image not found</div> <div>Dichloromethane</div> <div>Measured: 2.27</div> <div>Predicted: 2.41</div>	